

Charge and energy transport at the nanoscale: A DFT perspective

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Understanding the interplay between charge and energy transport at the nanoscale paves the way for novel thermoelectric devices, which may prove useful for the development for sustainable energy sources. However, concepts, such as heat flow, temperature and entropy are only well-established at the macroscopic level for slow dynamics. This raises

the question about whether these concepts can be employed for small length and short time scales. We will present our recent efforts to use a time-dependent density-functional theory framework, dubbed thermal DFT, in order to generalize temperature and heat or energy flow to the microscopic regime. To this end we will highlight the analogy of the formally exact microscopic equations of motion for charge density and energy density in thermal DFT to the macroscopic equations of motion of hydrodynamics. Furthermore, we will present first result using our approach to compute transient energy energy currents induced by a temperature gradient and show that in the steady-state limit persistent temperature oscillations develop.

This project has received funding from the European Union's Framework Programme for Research and Innovation Horizon 2020 (2014-2020) under the Marie Skłodowska-Curie Grant Agreement No. 701796.